

ATOMS CONFINED BY VERY THIN LAYERS

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ABSTRACT. We consider the Hamiltonian of an atom with N electrons and a fixed nucleus in a very thin plane-parallel layer. Projecting this Hamiltonian on the lowest transverse mode we obtain the so-called effective Hamiltonian that acts on $L^2(\mathbb{R}^{2N})$ and whose potential part depends on the width, a , of the layer. We prove that this effective Hamiltonian tends, in the norm resolvent sense, to the Hamiltonian of a two-dimensional atom (with the three-dimensional Coulomb potential) as $a \rightarrow 0+$. Finally we demonstrate how to localize the bottom of spectrum of the initial full Hamiltonian with the knowledge of the spectrum of the latter one. The analyticity and the monotonicity of eigenvalues in a is also discussed.

1. INTRODUCTION

In this paper we discuss a non-relativistic quantum system of an atom confined in a thin planar layer of width a . We describe it by the three-dimensional atomic Hamiltonian restricted to the layer, i.e., we impose the Dirichlet boundary condition on the boundary planes. The study of confined atomic systems has a long history ([15], from 1937, and [5], from 1946, deal with the hydrogen atom with a nucleus placed at the center of an impenetrable spherical box of finite radius), as these systems may serve as important models for caged and compressed atoms (see e.g. [7, 10, 13, 12]) or hydrogenic impurities in quantum dots (see e.g. [23, 14]). In the references above only the confinement to finite regions, usually to balls, is considered. However, with prospects of mesoscopic physics applications and for richer mathematical properties of respective Hamiltonians (presence of the continuous spectrum), a hydrogen atom confined in regions that are unbounded in some directions has recently drawn interest.

Namely, [4] is devoted to a hydrogen atom confined in a straight infinite tube, whereas in [6] a hydrogen atom in a thin planar layer of width a was studied. The present paper may be viewed as an extension of the results obtained in the latter source to a multi-electron case. Therein the so-called effective Hamiltonian was introduced as a projection of the full Hamiltonian to the lowest transverse mode of the Dirichlet Laplacian on the layer. Due to the large separation distance between subsequent eigenvalues of the Dirichlet Laplacian in the transverse direction ($\propto a^{-2}$), it was demonstrated that the effective Hamiltonian well approximates the full atomic Hamiltonian in the norm resolvent sense as $a \rightarrow 0+$. The effective Hamiltonian may be, in turn, approximated by the Hamiltonian of a two-dimensional hydrogen atom (with the three-dimensional Coulomb potential, i.e. $1/\text{distance}$) as $a \rightarrow 0+$. As the spectrum of the latter Hamiltonian is explicitly known, one can use it to approximate the spectrum of the full Hamiltonian.

Let us stress that there are several new aspects that complicates a similar analysis in the multi-electron case. First of all the repulsive electron to electron interaction is

involved, but fortunately it can be controlled in similar way as the electron to nucleus interaction with the appropriate change of coordinates. Next we must take the fermionic nature of electrons into the account. Actually we will treat electrons as distinguishable particles and only at the end of the paper we perform reduction to the subspace of totally antisymmetric functions. Finally, let us mention that the spectrum of a two-dimensional (as well as a three-dimensional) atom is not known explicitly except of the single electron case. Nevertheless, there are some qualitative results for two-dimensional atoms, in particular we will need the HVZ theorem. (See [17] for it. Zhislin's theorem and the asymptotic neutrality is discussed in the same source too.)

The paper is organized as follows. In sections 2, 3, and 4, the Hamiltonians of a two-dimensional atom and an atom in a planar layer, and the effective Hamiltonian, respectively, are introduced in detail and their self-adjointness is verified. In the next sections, we set the relation between these Hamiltonians. The main theorem comes in section 7, it claims that the full Hamiltonian is well approximated by the Hamiltonian of a two-dimensional atom as $a \rightarrow 0+$. Therefore the two-dimensional atom, which is a kind of mathematical construction, may be viewed as a limit of a physical system of an atom compressed among a pair of parallel planes. In this context, let us remark that the two-dimensional hydrogen atom (with the three-dimensional Coulomb potential) is of continuous interest in the literature (see e.g., [16, 21, 3, 8]), and here we provide rationale for it.

Section 8 is devoted to localization of the point spectrum of the full Hamiltonian and to analyticity of its eigenvalues in a . In the last, 9th, section we discuss the fermionized versions of the Hamiltonians and we conclude that the approximation results remain valid.

2. HAMILTONIAN OF A TWO-DIMENSIONAL ATOM

Consider N mutually interacting electrons with the unit charge and mass in the field of a nucleus with the atomic charge $Z > 0$ and the infinite mass. Denote by $\boldsymbol{\varrho}_i \equiv (x_i, y_i)$ the coordinate of the i th electron in the center of mass coordinate system and introduce the following notation

$$\varrho_i = |\boldsymbol{\varrho}_i|, \quad \varrho_{i,j} = |\boldsymbol{\varrho}_i - \boldsymbol{\varrho}_j|.$$

Then the Hamiltonian of the system, $h_{Z,N}$, is given by

$$h_{N,Z} = \sum_{i=1}^N -\Delta_{\boldsymbol{\varrho}_i} - \sum_{i=1}^N \frac{Z}{\varrho_i} + \sum_{1 \leq i < j \leq N} \frac{1}{\varrho_{i,j}}$$

$$Q(h_{N,Z}) = \mathcal{H}^1(\mathbb{R}^2)^{\otimes N} \equiv \mathcal{H}^1(\mathbb{R}^{2N})$$

where $\Delta_{\boldsymbol{\varrho}_i}$ stands for the Laplacian in the i th coordinate (naturally extended on the appropriate tensor product that is obvious from the context). Below we will prove that, due to the KLMN theorem, $h_{N,Z}$ is a well defined lower bounded self-adjoint operator.

Lemma 2.1. *For any $\psi \in \mathcal{H}^1(\mathbb{R}^4)$, it holds*

$$\langle \psi, \varrho_{i,j}^{-1} \psi \rangle \leq \frac{\Gamma(1/4)^4}{4\pi^2 \sqrt{2}} \langle \psi, \sqrt{-\Delta_{\boldsymbol{\varrho}_i} - \Delta_{\boldsymbol{\varrho}_j}} \psi \rangle.$$

Proof. With the aid of an unitary mapping $U : L^2(\mathbb{R}^4) \rightarrow L^2(\mathbb{R}^4)$,

$$(U\psi)(\mathbf{s}, \mathbf{t}) = \psi\left(\frac{\mathbf{s}-\mathbf{t}}{\sqrt{2}}, \frac{\mathbf{s}+\mathbf{t}}{\sqrt{2}}\right),$$

and the two-dimensional Kato inequality (see [9], [1]),

$$\frac{1}{\varrho} \leq \frac{\Gamma(1/4)^4}{4\pi^2} \sqrt{-\Delta_{\varrho}}, \quad \text{in } \mathcal{H}^1(\mathbb{R}^2),$$

we have

$$(1) \quad \begin{aligned} \langle \psi, \varrho_{i,j}^{-1} \psi \rangle &= \langle U\psi, U\varrho_{i,j}^{-1}U^\dagger U\psi \rangle \\ &\leq \frac{\Gamma(1/4)^4}{4\pi^2\sqrt{2}} \int_{\mathbb{R}^4} \psi\left(\frac{\mathbf{s}-\mathbf{t}}{\sqrt{2}}, \frac{\mathbf{s}+\mathbf{t}}{\sqrt{2}}\right)^* \sqrt{-\Delta_{\mathbf{t}}} \psi\left(\frac{\mathbf{s}-\mathbf{t}}{\sqrt{2}}, \frac{\mathbf{s}+\mathbf{t}}{\sqrt{2}}\right) d\mathbf{s} d\mathbf{t}. \end{aligned}$$

Since the minus Laplacian is a positive operator,

$$(2) \quad -\Delta_{\mathbf{t}} \leq -\Delta_{\mathbf{t}} - \Delta_{\mathbf{s}} = -\Delta_{\varrho_i} - \Delta_{\varrho_j}.$$

The same inequality holds for the square roots due to the operator monotonicity of the function $x \mapsto x^p$, $0 < p \leq 1$. Passing back to the variables (ϱ_i, ϱ_j) in (1), the assertion of the lemma follows. \square

Proposition 2.2. *Denote*

$$\mathcal{V}_{2D} = -\sum_{i=1}^N \frac{Z}{\varrho_i} + \sum_{1 \leq i < j \leq N} \frac{1}{\varrho_{i,j}}.$$

Then for any $\epsilon > 0$ and $\psi \in H^1(\mathbb{R}^{2N})$,

$$|\langle \psi, \mathcal{V}_{2D} \psi \rangle| \leq \frac{\Gamma(1/4)^4}{8\pi^2} \sqrt{N} \max\left\{\frac{N-1}{\sqrt{2}}, Z\right\} (\epsilon \|\nabla \psi\|^2 + \epsilon^{-1} \|\psi\|^2)$$

and

$$(3) \quad \inf \Theta(h_{N,Z}) \geq -\left(\frac{\Gamma(1/4)^4}{8\pi^2} \sqrt{N} Z\right)^2.$$

Proof. Let $\hat{\psi}$ (with the variable $\boldsymbol{\lambda} \equiv (\lambda_1, \dots, \lambda_N)$) stands for the Fourier-Plancherel image of ψ . Then by the two-dimensional Kato inequality,

$$(4) \quad \begin{aligned} -\langle \psi, \mathcal{V}_{2D} \psi \rangle &\leq \langle \psi, Z \sum_i \varrho_i^{-1} \psi \rangle \leq \frac{\Gamma(1/4)^4}{4\pi^2} Z \langle \hat{\psi}, \sum_i |\lambda_i| \hat{\psi} \rangle \leq \frac{\Gamma(1/4)^4}{4\pi^2} Z \langle \hat{\psi}, \sqrt{N} |\boldsymbol{\lambda}| \hat{\psi} \rangle \\ &\leq \frac{\Gamma(1/4)^4}{4\pi^2} Z \sqrt{N} \|\psi\| \|\nabla \psi\| \leq \frac{\Gamma(1/4)^4}{8\pi^2} Z \sqrt{N} (\epsilon \|\nabla \psi\|^2 + \epsilon^{-1} \|\psi\|^2). \end{aligned}$$

Using Lemma 2.1 we obtain in a similar manner as above,

$$\begin{aligned} \langle \psi, \mathcal{V}_{2D} \psi \rangle &\leq \langle \psi, \sum_{i < j} \varrho_{i,j}^{-1} \psi \rangle \leq \frac{\Gamma(1/4)^4}{4\pi^2\sqrt{2}} \langle \hat{\psi}, \sum_{i < j} \sqrt{\lambda_i^2 + \lambda_j^2} \hat{\psi} \rangle \\ &\leq \frac{\Gamma(1/4)^4}{4\pi^2\sqrt{2}} (N-1) \langle \hat{\psi}, \sum_i |\lambda_i| \hat{\psi} \rangle \leq \frac{\Gamma(1/4)^4}{8\pi^2\sqrt{2}} (N-1) \sqrt{N} (\epsilon \|\nabla \psi\|^2 + \epsilon^{-1} \|\psi\|^2). \end{aligned}$$

Neglecting the positive part of \mathcal{V}_{2D} , the lower bound (3) follows from the KLMN theorem. \square

Remark 2.3 (Spectrum of $h_{N,Z}$). *The spectrum of $h_{N,Z}$ is of course explicitly known only if $N = 1$. In that case [25, 6],*

$$\sigma_p(h_{1,Z}) = \left\{ -\frac{Z^2}{(2N-1)^2}, N \in \mathbb{N} \right\}, \quad \sigma_{ess}(h_{1,Z}) = \sigma_{ac}(h_{1,Z}) = [0, \infty).$$

For $N > 1$ we have at least HVZ theorem (see [22], [17]) which states that

$$\sigma_{ess}(h_{N,Z}) = [\inf \sigma(h_{N-1,Z}), \infty).$$

See [17] for some more results.

3. HAMILTONIAN OF AN ATOM IN A LAYER

Let $\Omega_a = \mathbb{R}^2 \times (-a/2, a/2)$ with $a > 0$. Consider a three-dimensional atom with N electrons and with a nucleus of the infinite mass and of the charge $Z > 0$ restricted to Ω_a by imposing the Dirichlet boundary condition on the boundary planes. For simplicity let us put the nucleus to the origin. Then the Hamiltonian, $H_{N,Z}^a$, of this system acts on $L^2(\Omega_a)^{\otimes N}$ as follows,

$$H_{N,Z}^a = -\Delta - \sum_{i=1}^N \frac{Z}{r_i} + \sum_{1 \leq i < j \leq N} \frac{1}{r_{i,j}},$$

where $\mathbf{r}_i \equiv (x_i, y_i, z_i) \in \Omega_a$ is the coordinate of the i th electron,

$$r_i = |\mathbf{r}_i|, \quad r_{i,j} = |\mathbf{r}_i - \mathbf{r}_j|,$$

and $-\Delta$ is the free Hamiltonian of N -particle system. In more detail,

$$-\Delta = -\sum_{i=1}^N \mathbb{I} \otimes \dots \otimes \Delta_{\mathbf{r}_i} \otimes \dots \otimes \mathbb{I}$$

$$\text{Dom}(-\Delta) = (\mathcal{H}_0^1(\Omega_a) \cap \mathcal{H}^2(\Omega_a))^{\otimes N},$$

where $\Delta_{\mathbf{r}_i}$ is the Laplace operator on $L^2(\Omega_a)$ (in the variable \mathbf{r}_i) with the Dirichlet boundary condition. Below we will find the domain of self-adjointness of $H_{N,Z}^a$.

Put

$$\mathcal{V} = -\sum_{i=1}^N \frac{Z}{r_i} + \sum_{1 \leq i < j \leq N} \frac{1}{r_{i,j}}.$$

Then

$$\|\mathcal{V}\psi\|^2 \leq Z^2 N \sum_{i=1}^N \|r_i^{-1}\psi\|^2 + \binom{N}{2} \sum_{1 \leq i < j \leq N} \|r_{i,j}^{-1}\psi\|^2.$$

Take $\psi \in (\mathcal{H}_0^1(\Omega_a) \cap \mathcal{H}^2(\Omega_a))^{\otimes N}$. Recall that the Hardy inequality (see e.g. [24]) states

$$(5) \quad \frac{1}{4} \int_{\mathbb{R}^3} \frac{|u(\mathbf{x})|^2}{|\mathbf{x}|^2} d\mathbf{x} \leq \int_{\mathbb{R}^3} |\nabla u(\mathbf{x})|^2 d\mathbf{x}$$

for any $u \in \mathcal{D}^{1,2}(\mathbb{R}^3)$, and that $\mathcal{H}_0^1(\Omega_a)$ may be naturally embedded into $\mathcal{D}^{1,2}(\mathbb{R}^3)$. Thus we have

$$\|r_i^{-1}\psi\|^2 \leq 4\|\nabla_{\mathbf{r}_i}\psi\|^2 = 4\langle\psi, -\Delta_{\mathbf{r}_i}\psi\rangle.$$

Similarly we obtain

$$\begin{aligned} \|r_{1,2}^{-1}\psi\|^2 &= \int_{\Omega_a^{\times N}} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|^2} |\psi(\mathbf{r}_1, \dots, \mathbf{r}_N)|^2 d\mathbf{r}_1 \dots d\mathbf{r}_N \\ &= \int_{\Omega_a^{\times (N-1)}} \int_{\mathbb{R}^2 \times (-a/2-t_z, a/2-t_z)} \frac{1}{|\mathbf{u}|^2} |\psi(\mathbf{u} + \mathbf{t}, \mathbf{t}, \mathbf{r}_3, \dots, \mathbf{r}_N)|^2 d\mathbf{u} d\mathbf{t} d\mathbf{r}_3 \dots d\mathbf{r}_N \\ &\leq 4 \int_{\Omega_a^{\times (N-1)}} \int_{\mathbb{R}^2 \times (-a/2-t_z, a/2-t_z)} |\nabla_{\mathbf{u}}\psi(\mathbf{u} + \mathbf{t}, \mathbf{t}, \mathbf{r}_3, \dots, \mathbf{r}_N)|^2 d\mathbf{u} d\mathbf{t} d\mathbf{r}_3 \dots d\mathbf{r}_N \\ &= 4 \int_{\Omega_a^{\times N}} |\nabla_{\mathbf{r}_1}\psi(\mathbf{r}_1, \dots, \mathbf{r}_N)|^2 d\mathbf{r}_1 \dots d\mathbf{r}_N = 4\langle\psi, -\Delta_{\mathbf{r}_1}\psi\rangle. \end{aligned}$$

Here t_z stands for the z -component of vector \mathbf{t} .

We conclude that

$$\begin{aligned} (6) \quad \|\mathcal{V}\psi\|^2 &\leq 4 \left(Z^2 N + \binom{N}{2} (N-1) \right) \langle\psi, -\Delta\psi\rangle \\ &\leq (2Z^2 N + N(N-1)^2) \left(\epsilon^2 \|\psi\|^2 + \epsilon^{-2} \|\psi\|^2 \right) \end{aligned}$$

for any $\epsilon > 0$. Hence $H_{N,Z}^a$ is self-adjoint on

$$\text{Dom}(H_{N,Z}^a) = \text{Dom}(-\Delta) = (\mathcal{H}_0^1(\Omega_a) \cap \mathcal{H}^2(\Omega_a))^{\otimes N}$$

by the Kato-Rellich theorem.

4. THE EFFECTIVE HAMILTONIAN

Decompose the kinetic part of $H_{N,Z}^a$ with respect to the transverse modes,

$$-\Delta = \sum_{i=1}^N -\Delta_{\mathbf{r}_i} = \sum_{i=1}^N \left[\bigoplus_{n=1}^{\infty} (-\Delta_{\mathbf{e}_i} + E_n^a) \otimes \langle \cdot, \chi_n^a \rangle \chi_n^a \right],$$

where $E_n^a = (n\pi/a)^2$ and

$$\chi_n^a(z) = \sqrt{\frac{2}{a}} \begin{cases} \cos \frac{n\pi z}{a} & \text{if } n \text{ is odd} \\ \sin \frac{n\pi z}{a} & \text{if } n \text{ is even.} \end{cases}$$

The effective Hamiltonian, H_{eff}^a , is defined with the aid of the projection on the lowest transverse mode,

$$P^a = \bigotimes_{i=1}^N [\mathbb{I}_{\mathbb{R}^2} \otimes \langle \cdot, \chi_1^a(z_i) \rangle \chi_1^a(z_i)],$$

as

$$H_{\text{eff}}^a = P^a H_{N,Z}^a P^a.$$

It is well defined on $\text{Dom}(H_{N,Z}^a)$ as $\text{Dom}(H_{N,Z}^a)$ is invariant under P^a . Moreover, $P^a \text{Dom}(H_{N,Z}^a)$ is naturally isometric to $\mathcal{H}^2(\mathbb{R}^2)^{\otimes N}$. Thus we will view H_{eff}^a as an operator on $L^2(\mathbb{R}^{2N})$ with the following action

$$H_{\text{eff}}^a = \sum_{i=1}^N -\Delta_{\varrho_i} + NE_1^a - Z \sum_{i=1}^N V_{en}^a(\varrho_i) + \sum_{1 \leq i < j \leq N} V_{ee}^a(\varrho_{i,j})$$

and with domain $\mathcal{H}^2(\mathbb{R}^2)^{\otimes N}$. Here the “effective potentials” are defined by

$$V_{en}^a(\varrho) = \frac{4}{a} \int_0^{a/2} \frac{\cos^2 \frac{\pi s}{a}}{\sqrt{\varrho^2 + s^2}} ds,$$

$$V_{ee}^a(\varrho) = \frac{4}{a^2} \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} \frac{\cos^2 \frac{\pi s}{a} \cos^2 \frac{\pi t}{a}}{\sqrt{\varrho^2 + (s-t)^2}} ds dt.$$

Below we will prove self-adjointness of H_{eff}^a . At first we need to know L^p -properties of the effective potentials.

The properties of V_{en}^a are extensively discussed in [6] (therein V_{en}^a is called V_{eff}^a), but we will also summarize some of them here for the reader's convenience. At the same time, for V_{ee}^a one directly verifies,

Asymptotic behavior

$$V_{ee}^a(\varrho) = \frac{1}{\varrho} + O\left(\frac{1}{\varrho^3}\right) \quad \text{as } \varrho \rightarrow \infty \quad (\text{the same as for } V_{en}^a)$$

$$V_{ee}^a(\varrho) = -\frac{3}{a} \ln \varrho + O(1) \quad \text{as } \varrho \rightarrow 0 + \quad (\text{the leading term for } V_{en}^a \text{ is } -\frac{4}{a} \ln \varrho)$$

Scaling properties

$$V_{ee}^a(\varrho) = \frac{1}{a} V_{ee}^1\left(\frac{\varrho}{a}\right) \quad (\text{the same as for } V_{en}^a)$$

Bounds

$$(7) \quad 0 \leq V_{ee}^a(\varrho) \leq \frac{1}{\varrho} \quad (\text{the same as for } V_{en}^a).$$

Moreover V_{ee}^a is strictly decreasing.

With these results in hand, it is easy to see that the potential W_{ee} defined by $W_{ee}(\varrho) = 1 - \varrho V_{ee}^1(\varrho)$ is $L^1(\mathbb{R}_+, d\varrho)$ -function and $0 \leq W_{ee} \leq 1$. The same holds for W_{en} defined just by interchanging $ee \leftrightarrow en$. Consequently, we can apply [6, Lemma 5] to them. Here we reproduce this result in a slightly modified form.

Lemma 4.1. *Suppose $W \in L^1(\mathbb{R}_+, d\varrho)$ and $0 \leq W \leq 1$. Put*

$$(8) \quad V^a(\varrho) = \frac{1}{\varrho} \left(1 - W\left(\frac{\varrho}{a}\right)\right), \quad a > 0.$$

Then for any a , $0 < a < 1/2$, one has

$$(9) \quad \begin{aligned} & \|(-\Delta_{2D} + 2)^{-1/2} (\varrho^{-1} - V^a) (-\Delta_{2D} + 2)^{-1/2}\| \\ & \leq 2\sqrt{3} a |\ln a| \int_{\mathbb{R}_+} W(\varrho) d\varrho + 4\sqrt{2} a \left(\int_{\mathbb{R}_+} W(\varrho) d\varrho \right)^{1/2}. \end{aligned}$$

Above Δ_{2D} stands for the two-dimensional Laplacian.

Furthermore, one can easily observe that

$$V_{en}^a, V_{ee}^a \in L^2(\mathbb{R}^2) + L^\infty(\mathbb{R}^2).$$

Hence in the similar manner as in the three-dimensional case (see [18, Theo X.16]) it follows that H_{eff}^a is self-adjoint on $\mathcal{H}^2(\mathbb{R}^2)^{\otimes N}$ due to the Kato-Rellich theorem.

Remark 4.2 (Spectrum of H_{eff}^a). *Due to (7), $\sigma(H_{\text{eff}}^a - NE_1^a)$ has a lower bound given by the RHS of (3). Moreover from the HVZ theorem follows that $[NE_1^a, \infty) \subset \sigma_{\text{ess}}(H_{\text{eff}}^a)$.*

5. APPROXIMATION OF THE EFFECTIVE HAMILTONIAN BY THE TWO-DIMENSIONAL ATOMIC HAMILTONIAN

Observe that single-particle potentials that are controlled by the two-dimensional free particle Hamiltonian, $-\Delta_{2D}$, are also controlled by the full free Hamiltonian, $-\Delta$. The same holds true for electron-to-electron interaction terms (that are only functions of the mutual distance) as they may be viewed as single-particle potentials with the appropriate change of coordinates. Indeed, for $\xi > 0$,

$$(-\Delta_{2D} + \xi) \otimes \mathbb{I} \leq -\Delta + \xi$$

which implies

$$(-\Delta + \xi)^{-1} \leq (-\Delta_{2D} + \xi)^{-1} \otimes \mathbb{I},$$

since the function $x \mapsto -x^{-1}$ is operator monotone. In particular for all $\psi \in Q(V \otimes \mathbb{I})$, where $V \geq 0$ and $Q(V) = Q(-\Delta_{2D}) = \mathcal{H}^1(\mathbb{R}^2)$,

$$\langle \psi, \sqrt{V \otimes \mathbb{I}} (-\Delta + \xi)^{-1} \sqrt{V \otimes \mathbb{I}} \psi \rangle \leq \langle \psi, [\sqrt{V} (-\Delta_{2D} + \xi)^{-1} \sqrt{V}] \otimes \mathbb{I} \psi \rangle$$

from which it follows

$$\|\sqrt{V \otimes \mathbb{I}} (-\Delta + \xi)^{-1} \sqrt{V \otimes \mathbb{I}}\| \leq \|\sqrt{V} (-\Delta_{2D} + \xi)^{-1} \sqrt{V}\|$$

or equivalently

$$(10) \quad \|(-\Delta + \xi)^{-1/2} (V \otimes \mathbb{I}) (-\Delta + \xi)^{-1/2}\| \leq \|(-\Delta_{2D} + \xi)^{-1/2} V (-\Delta_{2D} + \xi)^{-1/2}\|.$$

Let us denote

$$\mathcal{V}^a = Z \sum_{i=1}^N \left(\frac{1}{\varrho_i} - V_{en}^a(\varrho_i) \right) - \sum_{1 \leq i < j \leq N} \left(\frac{1}{\varrho_{i,j}} - V_{ee}^a(\varrho_{i,j}) \right).$$

Then with the aid of the above, we get the following proposition.

Proposition 5.1. *For any $0 < a < 1/2$, we have*

$$(11) \quad \begin{aligned} & \|(-\Delta + 2)^{-1/2} |\mathcal{V}^a| (-\Delta + 2)^{-1/2}\| \\ & \leq 2\sqrt{3} \left[ZN \left(\frac{1}{4} - \frac{1}{\pi^2} \right) + \binom{N}{2} \left(\frac{1}{3} - \frac{5}{4\pi^2} \right) \right] a |\ln a| \\ & \quad + 4\sqrt{2} \left[ZN \left(\frac{1}{4} - \frac{1}{\pi^2} \right)^{1/2} + \binom{N}{2} \left(\frac{1}{3} - \frac{5}{4\pi^2} \right)^{1/2} \right] a. \end{aligned}$$

Proof. By the triangle inequality and (10),

$$\begin{aligned} & \|(-\Delta + 2)^{-1/2} |\mathcal{V}^a| (-\Delta + 2)^{-1/2}\| \\ & \leq ZN \left\| (-\Delta_{\varrho_1} + 2)^{-1/2} (\varrho_1^{-1} - V_{en}^a(\varrho_1)) (-\Delta_{\varrho_1} + 2)^{-1/2} \right\| \\ & \quad + \binom{N}{2} \left\| (-\Delta_{\varrho_1} - \Delta_{\varrho_2} + 2)^{-1/2} (\varrho_{1,2}^{-1} - V_{ee}^a(\varrho_{1,2})) (-\Delta_{\varrho_1} - \Delta_{\varrho_2} + 2)^{-1/2} \right\|. \end{aligned}$$

In the second term we may estimate with the aid of (2) ($\mathbf{t} = 2^{-1/2} \varrho_{1,2}$) as follows,

$$\begin{aligned} & \left\| (-\Delta_{\varrho_1} - \Delta_{\varrho_2} + 2)^{-1/2} (\varrho_{1,2}^{-1} - V_{ee}^a(\varrho_{1,2})) (-\Delta_{\varrho_1} - \Delta_{\varrho_2} + 2)^{-1/2} \right\| \\ & \leq \left\| (-\Delta_{\mathbf{t}} + 2)^{-1/2} (\varrho_{1,2}^{-1} - V_{ee}^a(\varrho_{1,2})) (-\Delta_{\mathbf{t}} + 2)^{-1/2} \right\|. \end{aligned}$$

Since

$$\|(-\Delta_{\varrho_{1,2}} + 2)^{1/2} (-\Delta_{\mathbf{t}} + 2)^{-1/2}\|^2 = \frac{1}{2} \|(-\Delta_{\varrho_{1,2}} + 2)^{1/2} (-\Delta_{\varrho_{1,2}} + 1)^{-1/2}\|^2 = 1,$$

we obtain

$$\begin{aligned} & \|(-\Delta_{\varrho_1} - \Delta_{\varrho_2} + 2)^{-1/2} (\varrho_{1,2}^{-1} - V_{ee}^a(\varrho_{1,2})) (-\Delta_{\varrho_1} - \Delta_{\varrho_2} + 2)^{-1/2}\| \\ & \leq \|(-\Delta_{\varrho_{1,2}} + 2)^{-1/2} (\varrho_{1,2}^{-1} - V_{ee}^a(\varrho_{1,2})) (-\Delta_{\varrho_{1,2}} + 2)^{-1/2}\|. \end{aligned}$$

Now we may use Lemma 4.1 which yields

$$\begin{aligned} & \|(-\Delta + 2)^{-1/2} |\mathcal{V}^a| (-\Delta + 2)^{-1/2}\| \\ & \leq 2\sqrt{3} \left[ZN \left(\int_{\mathbb{R}_+} W_{en}(\varrho) d\varrho \right) + \binom{N}{2} \left(\int_{\mathbb{R}_+} W_{ee}(\varrho) d\varrho \right) \right] a |\ln a| \\ & \quad + 4\sqrt{2} \left[ZN \left(\int_{\mathbb{R}_+} W_{en}(\varrho) d\varrho \right)^{1/2} + \binom{N}{2} \left(\int_{\mathbb{R}_+} W_{ee}(\varrho) d\varrho \right)^{1/2} \right] a. \end{aligned}$$

The integrals of W_{en} and W_{ee} may be evaluated using Fubini's theorem,

$$\begin{aligned} \int_{\mathbb{R}_+} W_{en}(\varrho) d\varrho &= \frac{1}{4} - \frac{1}{\pi^2} \\ \int_{\mathbb{R}_+} W_{ee}(\varrho) d\varrho &= \frac{1}{3} - \frac{5}{4\pi^2}, \end{aligned}$$

which completes the proof. \square

Further we will need an estimate formulated in the following auxiliary lemma that in fact is a standard result (see for instance, [19, Chp. XI]).

Lemma 5.2. *Assume that A is semi-bounded, A^{-1} exists and is bounded, C is self-adjoint and A form bounded. If*

$$\alpha = \| |C|^{1/2} |A|^{-1/2} \| < 1$$

then $(A + C)^{-1}$ exists, is bounded and

$$\|(A + C)^{-1} - A^{-1}\| \leq \frac{\alpha^2 \|A^{-1}\|}{1 - \alpha^2}.$$

Theorem 5.3. *Let $d_{N,Z}(\xi)$ stands for the distance of ξ from $\sigma(h_{N,Z})$. Then for every $\xi \in \text{Res}(h_{N,Z}) \cap \mathbb{R}$ there exists $a_0(\xi) > 0$ (which is given within the proof) such that for all a , $0 < a < a_0(\xi)$, one has $\xi \in \text{Res}(H_{\text{eff}}^a - NE_1^a)$ and*

$$\begin{aligned} & \| (H_{\text{eff}}^a - NE_1^a - \xi)^{-1} - (h_{N,Z} - \xi)^{-1} \| \\ & \leq \frac{2}{d_{N,Z}(\xi)} \max \left\{ 1, \frac{-\mu}{d_{N,Z}(\xi)} \right\} C_1(N, Z)^2 C_2(N, Z) a |\ln a|, \end{aligned}$$

where $\mu \leq (\inf \sigma(h_{N,Z}) - 1)$. The constant $C_1(N, Z)$ and $C_2(N, Z)$ are given in (13) and (14), respectively.

Proof. In Lemma 5.2, we set

$$A = h_{N,Z} - \xi, \quad C = \mathcal{V}^a.$$

Then $\|A^{-1}\| = d_{N,Z}(\xi)^{-1}$ and

$$\begin{aligned} \alpha^2 &= \| |h_{N,Z} - \xi|^{-1/2} |\mathcal{V}^a| |h_{N,Z} - \xi|^{-1/2} \|^2 \leq \| (h_{N,Z} - \mu)^{1/2} |h_{N,Z} - \xi|^{-1/2} \|^2 \\ & \times \| (-\Delta - \mu)^{1/2} (h_{N,Z} - \mu)^{-1/2} \|^2 \| (-\Delta + 2)^{1/2} (-\Delta - \mu)^{-1/2} \|^2 \\ & \times \| (-\Delta + 2)^{-1/2} |\mathcal{V}^a| (-\Delta + 2)^{-1/2} \| \end{aligned}$$

where μ is chosen smaller than $(\inf \sigma(h_{N,Z}) - 1) > -\infty$ (due to the HVZ theorem $\mu \leq -2$).

With the aid of the functional calculus, we have

$$\| (-\Delta + 2)^{1/2} (-\Delta - \mu)^{-1/2} \| = 1$$

and

$$\| (h_{N,Z} - \mu)^{1/2} |h_{N,Z} - \xi|^{-1/2} \|^2 = \sup_{\lambda \in \sigma(h_{N,Z})} \frac{\lambda - \mu}{|\lambda - \xi|} \leq \max \left\{ 1, \frac{-\mu}{d_{N,Z}(\xi)} \right\}.$$

To find an upper bound for the norm of $L := (-\Delta - \mu)^{1/2} (h_{N,Z} - \mu)^{-1/2}$, we imitate the proof of Lemma 4 in [6] (but now the total Coulomb potential, \mathcal{V}_{2D} , changes its sign),

$$\begin{aligned} (12) \quad & \|L\psi\|^2 = \langle \psi, L^* L \psi \rangle = \|\psi\|^2 + \langle (h_{N,Z} - \mu)^{-1/2} \psi, (-\mathcal{V}_{2D}) (h_{N,Z} - \mu)^{-1/2} \psi \rangle \\ & \leq \|\psi\|^2 + \frac{\Gamma(1/4)^4}{4\pi^2} Z \sqrt{N} \langle (h_{N,Z} - \mu)^{-1/2} \psi, \sqrt{-\Delta} (h_{N,Z} - \mu)^{-1/2} \psi \rangle \\ & \leq \|\psi\|^2 + \frac{\Gamma(1/4)^4}{4\pi^2} Z \sqrt{N} \| (h_{N,Z} - \mu)^{-1/2} \psi \| \|L\psi\|. \end{aligned}$$

Here we made use of (4) and the fact that $\sqrt{-\Delta} \leq \sqrt{-\Delta - \mu}$, for $\mu < 0$. With our choice of μ this implies

$$\|L\|^2 \leq 1 + \frac{\Gamma(1/4)^4}{4\pi^2} Z \sqrt{N} \|L\|.$$

So we have that

$$(13) \quad \|L\| \leq C_1(N, Z) := \frac{1}{8\pi^2} \left(\Gamma \left(\frac{1}{4} \right)^4 Z \sqrt{N} + \sqrt{\Gamma \left(\frac{1}{4} \right)^8 Z^2 N + 64\pi^4} \right).$$

Using Proposition 5.1, we conclude

$$\alpha^2 \leq \max \left\{ 1, \frac{-\mu}{d_{N,Z}(\xi)} \right\} C_1(N, Z)^2 \times [\text{RHS of (11)}].$$

Moreover, for $a \leq e^{-1}$, we have

$$\text{RHS of (11)} \leq C_2(N, Z)a|\ln a|$$

with

$$(14) \quad C_2(N, Z) := (2\sqrt{3} + 4\sqrt{2}) \left[ZN \left(\frac{1}{4} - \frac{1}{\pi^2} \right) + \binom{N}{2} \left(\frac{1}{3} - \frac{5}{4\pi^2} \right) \right].$$

For any $\xi \in \text{Res}(h_{N,Z}) \cap \mathbb{R}$, there is $a_0 = a_0(\xi)$ such that for all a , $0 < a < a_0(\xi)$, one has $\alpha^2 \leq 1/2$. For definiteness, we put

$$(15) \quad \mu = -N \left(\frac{\Gamma(1/4)^4 Z}{8\pi^2} \right)^2 - 1,$$

and we set $a_0(\xi) = \min \{e^{-1}, \tilde{a}_0(\xi)\}$, where $\tilde{a}_0 = \tilde{a}_0(\xi)$ is the solution to

$$(16) \quad \max \left\{ 1, \frac{-\mu}{d_{N,Z}(\xi)} \right\} C_1(N, Z)^2 C_2(N, Z) \tilde{a}_0 |\ln \tilde{a}_0| = 1/2.$$

The assertions of the theorem now immediately follow from Lemma 5.2. \square

Remark 5.4. *Under the assumptions of Theorem 5.3, we have*

$$\|(H_{\text{eff}}^a - NE_1^a - \xi)^{-1} - (h_{N,Z} - \xi)^{-1}\| \leq \|(h_{N,Z} - \xi)^{-1}\|,$$

which, by the functional calculus and the triangle inequality, implies

$$\frac{1}{d_{\text{eff}}(\xi + NE_1^a)} \leq \frac{2}{d_{N,Z}(\xi)},$$

with

$$(17) \quad d_{\text{eff}}(\xi) = \text{dist}(\xi, \sigma(H_{\text{eff}}^a)).$$

6. APPROXIMATION OF THE FULL HAMILTONIAN BY THE EFFECTIVE HAMILTONIAN

Let us introduce the following notation,

$$Q^a = 1 - P^a, \quad H_{\perp}^a = Q^a H_{N,Z}^a Q^a, \quad R_{\perp}^a(\xi) = (H_{\perp}^a - \xi)^{-1}.$$

Here, H_{\perp}^a is well defined on $\text{Dom}(H_{N,Z}^a)$ as $\text{Dom}(H_{N,Z}^a)$ is invariant under Q^a . In what follows we will view H_{\perp}^a as an operator acting on $\text{Ran} Q^a$ with domain $Q^a \text{Dom}(H_{N,Z}^a)$. Furthermore, put

$$\mathscr{W}^a(\xi) = P^a \mathcal{V} Q^a R_{\perp}^a(\xi) Q^a \mathcal{V} P^a, \quad R_{\text{eff}}^a(\xi) = (H_{\text{eff}}^a - \mathscr{W}^a(\xi) - \xi)^{-1},$$

where

$$\mathcal{V} = \mathcal{V}_{en} + \mathcal{V}_{ee}$$

with

$$\mathcal{V}_{en} = - \sum_{i=1}^N \frac{Z}{r_i}, \quad \mathcal{V}_{ee} = \sum_{1 \leq i < j \leq N} \frac{1}{r_{i,j}}.$$

With respect to the decomposition $L^2(\Omega_a)^{\otimes N} = \text{Ran}P^a \oplus \text{Ran}Q^a$, we have

$$H_{N,Z}^a = \begin{pmatrix} H_{\text{eff}}^a & P^a H_{N,Z}^a Q^a \\ Q^a H_{N,Z}^a P^a & H_{\perp}^a \end{pmatrix} = \begin{pmatrix} H_{\text{eff}}^a & P^a \mathcal{V} Q^a \\ Q^a \mathcal{V} P^a & H_{\perp}^a \end{pmatrix}$$

The second equality follows from the fact that P^a commutes with $-\Delta$. By direct inspection one arrives at the so-called Feshbach formula,

$$(18) \quad (H_{N,Z}^a - \xi)^{-1} = \begin{pmatrix} R_{\text{eff}}^{\mathcal{W}} & -R_{\text{eff}}^{\mathcal{W}} P^a \mathcal{V} Q^a R_{\perp}^a \\ -R_{\perp}^a Q^a \mathcal{V} P^a R_{\text{eff}}^{\mathcal{W}} & R_{\perp}^a + R_{\perp}^a Q^a \mathcal{V} P^a R_{\text{eff}}^{\mathcal{W}} P^a \mathcal{V} Q^a R_{\perp}^a \end{pmatrix},$$

which holds for those $\xi \in \mathbb{C}$ such that $R_{\perp}^a(\xi)$ and $R_{\text{eff}}^{\mathcal{W}}(\xi)$ exist and are bounded on $\text{Ran}Q^a$ and $\text{Ran}P^a$, respectively.

From now on, consider $N \geq 2$.

Proposition 6.1. *Let $0 < a < \sqrt{3}\pi/[2N(N-1+2Z)]$, $\xi < NE_1^a$, and $\xi \notin \sigma(H_{\text{eff}}^a - \mathcal{W}^a(\xi))$. Then $\xi \in \text{Res}(H_{N,Z}^a)$ and*

$$\|(H_{N,Z}^a - \xi)^{-1} - R_{\text{eff}}^{\mathcal{W}} \oplus 0\| \leq \frac{2Na}{\sqrt{3}\pi d_{\text{eff}}^{\mathcal{W}}(\xi)} (N-1+2Z) \left(1 + \frac{2Na}{\sqrt{3}\pi} (N-1+2Z)\right) + \frac{2a^2}{3\pi^2}.$$

where

$$d_{\text{eff}}^{\mathcal{W}}(\xi) = \text{dist}(\xi, \sigma(H_{\text{eff}}^a - \mathcal{W}^a(\xi))).$$

Proof. The proof is intensively inspired (as well as its single-electron version [6]) by the similar one in [2].

With the help of the following formula,

$$\left\| \begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix} \right\|^2 = \|AA^\dagger\| = \|A\|^2,$$

one derives the estimate

$$(19) \quad \begin{aligned} \|(H_{N,Z}^a - \xi)^{-1} - R_{\text{eff}}^{\mathcal{W}}(\xi) \oplus 0\| &\leq \|R_{\text{eff}}^{\mathcal{W}} P^a \mathcal{V} Q^a R_{\perp}^a\| + \|R_{\perp}^a Q^a \mathcal{V} P^a R_{\text{eff}}^{\mathcal{W}} P^a \mathcal{V} Q^a R_{\perp}^a\| + \|R_{\perp}^a\| \\ &\leq \frac{1}{d_{\text{eff}}^{\mathcal{W}}} \|\mathcal{V} Q^a R_{\perp}^a\| (1 + \|\mathcal{V} Q^a R_{\perp}^a\|) + \|R_{\perp}^a\|. \end{aligned}$$

It remains to bound $\|\mathcal{V} Q^a R_{\perp}^a\|$ and $\|R_{\perp}^a\|$.

Since

$$T_{\perp} := Q^a(-\Delta)Q^a \geq (N-1)E_1^a + E_2^a = NE_1^a + \frac{3\pi^2}{a^2},$$

we have

$$(20) \quad 0 \leq R_0 := (T_{\perp} - \xi)^{-1} \leq \frac{a^2}{3\pi^2}.$$

Further let us estimate $\|\mathcal{V} Q^a R_0^{1/2}\| = \|R_0^{1/2} Q^a \mathcal{V}^2 Q^a R_0^{1/2}\|^{1/2}$. As $\mathcal{V}^2 \leq \mathcal{V}_{en}^2 + \mathcal{V}_{ee}^2$, we can estimate the en and ee terms separately.

Bound for $\|\mathcal{V}_{en} Q^a R_0^{1/2}\|$: The following estimate,

$$\mathcal{V}_{en}^2 \leq \frac{Z^2}{2} \sum_{i,j} \left(\frac{1}{r_i^2} + \frac{1}{r_j^2} \right) = Z^2 N \sum_i \frac{1}{r_i^2}$$

together with the Hardy inequality (5), implies

$$\begin{aligned} R_0^{1/2} Q^a \mathcal{V}_{en}^2 Q^a R_0^{1/2} &\leq 4Z^2 N R_0^{1/2} Q^a (-\Delta) Q^a R_0^{1/2} = 4Z^2 N (Q^a + \xi R_0) \\ &\leq 4Z^2 N (1 + N/3) \leq 4Z^2 N^2, \end{aligned}$$

whenever $N \geq 2$, and so

$$(21) \quad \|\mathcal{V}_{en} Q^a R_0^{1/2}\| \leq 2ZN.$$

Bound for $\|\mathcal{V}_{ee} Q^a R_0^{1/2}\|$: In [2, Lemma 3.2] it was deduced that

$$\frac{1}{r_{i,j}^2} \leq 2(-\Delta_{\mathbf{r}_i} - \Delta_{\mathbf{r}_j})$$

in \mathbb{R}^3 . The same holds true in Ω_a . Using this inequality we have

$$\mathcal{V}_{ee}^2 \leq \frac{1}{2} \sum_{i < j, k < l} \left(\frac{1}{r_{i,j}^2} + \frac{1}{r_{k,l}^2} \right) \leq N(N-1) \sum_{i < j} (-\Delta_{\mathbf{r}_i} - \Delta_{\mathbf{r}_j}) = N(N-1)^2 (-\Delta),$$

and so, in the same manner as for the en part,

$$(22) \quad \|\mathcal{V}_{ee} Q^a R_0^{1/2}\| \leq N(N-1).$$

Bound for $\|R_\perp^a\|$: From (20), (21), and (22), it follows

$$\begin{aligned} (R_0^{1/2} Q^a \mathcal{V}_{en} Q^a R_0^{1/2})^2 &= R_0^{1/2} Q^a \mathcal{V}_{en} Q^a R_0 Q^a \mathcal{V}_{en} Q^a R_0^{1/2} \leq \frac{1}{3} \left(\frac{2ZN a}{\pi} \right)^2 \\ (R_0^{1/2} Q^a \mathcal{V}_{ee} Q^a R_0^{1/2})^2 &\leq \frac{1}{3} \left(\frac{N(N-1)a}{\pi} \right)^2, \end{aligned}$$

and consequently

$$\|R_0^{1/2} Q^a \mathcal{V} Q^a R_0^{1/2}\| \leq \frac{2ZN a}{\sqrt{3}\pi} + \frac{N(N-1)a}{\sqrt{3}\pi} = \frac{Na}{\sqrt{3}\pi} (N-1+2Z).$$

For a small enough, this bound is smaller than one, and so by the symmetrized resolvent formula,

$$(23) \quad R_\perp^a(\xi) = (T_\perp + Q^a \mathcal{V} Q^a - \xi)^{-1} = R_0^{1/2} \left(1 + R_0^{1/2} Q^a \mathcal{V} Q^a R_0^{1/2} \right)^{-1} R_0^{1/2},$$

one has $\xi \in \text{Res}(H_\perp^a)$ and the resolvent $R_\perp^a(\xi)$ is positive. Moreover,

$$\|R_\perp^a(\xi)\| \leq \frac{\|R_0\|}{1 - \|R_0^{1/2} Q^a \mathcal{V} Q^a R_0^{1/2}\|}.$$

For $a < \sqrt{3}\pi/[2N(N-1+2Z)]$,

$$(24) \quad \|R_\perp^a\| \leq 2\|R_0\| \leq \frac{2a^2}{3\pi^2}.$$

Bound for $\|\mathcal{V} Q^a R_\perp^a\|$: With the help of (23) (see also the proof of [6, Prop. 10]),

$$\|\mathcal{V} Q^a R_\perp^a\| \leq \frac{\|\mathcal{V} Q^a R_0^{1/2}\| \|R_\perp^a\|^{1/2}}{\left(1 - \|R_0^{1/2} Q^a \mathcal{V} Q^a R_0^{1/2}\|\right)^{1/2}} \leq \frac{2Na}{\sqrt{3}\pi} (N-1+2Z),$$

where we used (21), (22), and (24). \square

The following lemma is also generalization of its single-electron version (see [6, Lemma 11]).

Lemma 6.2. *Let $0 < a < \sqrt{3}\pi/[2N(N-1+2Z)]$. If $\xi < NE_1^a$, then $\mathscr{W}^a(\xi)$ is positive and*

$$\|(-\Delta + \alpha)^{-1/2} \mathscr{W}^a(\xi) (-\Delta + \alpha)^{-1/2}\| \leq \frac{\Gamma(1/4)^4 N^{3/2}}{6\pi^3 \sqrt{\alpha}} \left(Z^2 + \frac{(N-1)^2}{\sqrt{2}} \right) a$$

for any $\alpha > 0$.

Proof. In course of the proof of Proposition 6.1 we demonstrated that under the assumptions of the lemma, $R_\perp^a(\xi)$ is positive and so is $\mathscr{W}^a(\xi)$. Moreover, using (24) we get

$$\begin{aligned} 0 \leq \mathscr{W}^a(\xi) &= P^a \mathcal{V} Q^a R_\perp^a Q^a \mathcal{V} P^a \leq \frac{2a^2}{3\pi^2} P^a \mathcal{V}^2 P^a \leq \frac{2a^2}{3\pi^2} P^a (\mathcal{V}_{en}^2 + \mathcal{V}_{ee}^2) P^a \\ &\leq \frac{2a^2}{3\pi^2} \left(Z^2 N \sum_{i=1}^N P^a \frac{1}{r_i^2} P^a + \binom{N}{2} \sum_{1 \leq i < j \leq N} P^a \frac{1}{r_{i,j}^2} P^a \right). \end{aligned}$$

Since

$$P^a \frac{1}{r_i^2} P^a \leq \frac{2\pi}{a \varrho_i} \quad (\text{see [6, Lemma 11]})$$

and

$$\begin{aligned} P^a \frac{1}{r_{i,j}^2} P^a &= \frac{4}{a^2} \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} \frac{\cos^2 \frac{\pi s}{a} \cos^2 \frac{\pi t}{a}}{\varrho_{i,j}^2 + (s-t)^2} ds dt \leq \frac{4}{a^2} \int_{-a/2}^{a/2} \int_{-a/2-t}^{a/2-t} \frac{ds dt}{\varrho_{i,j}^2 + s^2} \\ &\leq \frac{8}{a} \int_0^\infty \frac{ds}{\varrho_{i,j}^2 + s^2} = \frac{4\pi}{a \varrho_{i,j}}, \end{aligned}$$

we conclude

$$\begin{aligned} \mathscr{W}^a(\xi) &\leq \frac{4Na}{3\pi} \left(Z^2 \sum_i \frac{1}{\varrho_i} + (N-1) \sum_{i < j} \frac{1}{\varrho_{i,j}} \right) \\ &\leq \frac{\Gamma(1/4)^4 Na}{3\pi^3} \left(Z^2 \sum_i \sqrt{-\Delta_{\mathbf{e}_i}} + \frac{N-1}{\sqrt{2}} \sum_{i < j} \sqrt{-\Delta_{\mathbf{e}_i} - \Delta_{\mathbf{e}_j}} \right) \end{aligned}$$

by the Kato inequality (see also Lemma 2.1).

Passing to the Fourier image (with the same notation as introduced in the proof of Proposition 2.2), we have

$$\begin{aligned} \langle \psi, \mathcal{W}^a(\xi) \psi \rangle &\leq \frac{\Gamma(1/4)^4 N a}{3\pi^3} \left\langle \hat{\psi}, \left(Z^2 \sum_i |\lambda_i| + \frac{N-1}{\sqrt{2}} \sum_{i < j} \sqrt{|\lambda_i|^2 + |\lambda_j|^2} \right) \hat{\psi} \right\rangle \\ &\leq \frac{\Gamma(1/4)^4 N a}{3\pi^3} \left(Z^2 + \frac{(N-1)^2}{\sqrt{2}} \right) \langle \hat{\psi}, \sum_i |\lambda_i| \hat{\psi} \rangle \\ &\leq \frac{\Gamma(1/4)^4 N^{3/2} a}{3\pi^3} \left(Z^2 + \frac{(N-1)^2}{\sqrt{2}} \right) \langle \psi, \sqrt{-\Delta} \psi \rangle. \end{aligned}$$

The lemma now readily follows, since

$$\|(-\Delta + \alpha)^{-1/2} \sqrt{-\Delta} (-\Delta + \alpha)^{-1/2}\| = \sup_{\lambda \in [0, \infty)} \frac{\sqrt{\lambda}}{\lambda + \alpha} = \frac{1}{2\sqrt{\alpha}}.$$

□

Proposition 6.3. *Suppose that $\xi \in \text{Res}(H_{\text{eff}}^a) \cap \mathbb{R}$. If $a \leq a_1(\xi)$ (with $a_1(\xi)$ introduced in the proof below), then $\xi \notin \sigma(H_{\text{eff}}^a - \mathcal{W}^a(\xi))$ and*

$$\|R_{\text{eff}}^{\mathcal{W}}(\xi) - (H_{\text{eff}}^a - \xi)^{-1}\| \leq \frac{2C_1(N, Z)^2}{d_{\text{eff}}(\xi)} \max \left\{ 1, \frac{-\mu}{d_{\text{eff}}(\xi)} \right\} \frac{\Gamma(1/4)^4 N^{3/2}}{6\pi^3 \sqrt{-\mu}} \left(Z^2 + \frac{(N-1)^2}{\sqrt{2}} \right) a,$$

where $d_{\text{eff}}(\xi)$ is defined by (17) and $\mu \leq \inf \sigma(H_{\text{eff}}^a) - NE_1^a - 1$.

Proof. Due to Remark 4.2, $\mu \leq -1$ and $\xi < NE_1^a$.

We will proceed as in the proof of Theorem 5.3. Apply Lemma 5.2 with $A = H_{\text{eff}}^a - \xi$, $C = -\mathcal{W}^a(\xi)$, i.e.,

$$\begin{aligned} \alpha^2 &= \| |H_{\text{eff}}^a - \xi|^{-1/2} \mathcal{W}^a |H_{\text{eff}}^a - \xi|^{-1/2} \| \\ (25) \quad &\leq \| (-\Delta - \mu)^{-1/2} \mathcal{W}^a (-\Delta - \mu)^{-1/2} \| \| (-\Delta - \mu)^{1/2} (H_{\text{eff}}^a - NE_1^a - \mu)^{-1/2} \|^2 \\ &\quad \times \| (H_{\text{eff}}^a - NE_1^a - \mu)^{1/2} |H_{\text{eff}}^a - \xi|^{-1/2} \|^2. \end{aligned}$$

Note that $\mathcal{W}^a(\xi)$ is positive under the assumptions of Lemma 6.2.

The upper bound for $\tilde{L} := (-\Delta - \mu)^{1/2} (H_{\text{eff}}^a - NE_1^a - \mu)^{-1/2}$ is the same as that for the operator L in the proof of Theorem 5.3. Indeed, since

$$-P^a \mathcal{V} P^a \leq P^a \mathcal{V}_{\text{en}} P^a \leq \sum_{i=1}^N \frac{Z}{\varrho_i}$$

we arrive at (12) with L replaced by \tilde{L} , \mathcal{V}_{2D} by $P^a \mathcal{V} P^a$, and $h_{N,Z}$ by H_{eff}^a . Consequently,

$$(26) \quad \|\tilde{L}\| = \|(-\Delta - \mu)^{1/2} (H_{\text{eff}}^a - NE_1^a - \mu)^{-1/2}\| \leq C_1(N, Z).$$

Furthermore we observe that

$$(27) \quad \| (H_{\text{eff}}^a - NE_1^a - \mu)^{1/2} |H_{\text{eff}}^a - \xi|^{-1/2} \|^2 \leq \max \left\{ 1, \frac{-\mu}{d_{\text{eff}}(\xi)} \right\}$$

by the functional calculus.

Putting (25), (26), (27), and Lemma 6.2 together, we deduce that there exists a positive $a_1 = a_1(\xi)$ such that if $a \leq a_1(\xi)$, then $\alpha^2 \leq 1/2$. This according to Lemma 5.2 implies that $\xi \notin \sigma(H_{\text{eff}}^a - \mathcal{W}^a(\xi))$ and

$$(28) \quad \|R_{\text{eff}}^{\mathcal{W}}(\xi) - (H_{\text{eff}}^a - \xi)^{-1}\| \leq \frac{2\alpha^2}{d_{\text{eff}}(\xi)}.$$

To make $a_1(\xi)$ definite we put, as in (15),

$$\mu = -N \left(\frac{\Gamma(1/4)^4 Z}{8\pi^2} \right)^2 - 1.$$

and define $a_1(\xi)$ as the unique solution of

$$(29) \quad \frac{\Gamma(1/4)^4 N^{3/2}}{6\pi^3 \sqrt{-\mu}} \left(Z^2 + \frac{(N-1)^2}{\sqrt{2}} \right) \max \left\{ 1, \frac{-\mu}{d_{\text{eff}}(\xi)} \right\} C_1(N, Z)^2 a_1 = \frac{1}{2}.$$

□

Theorem 6.4. *Let $\xi \in \text{Res}(H_{\text{eff}}^a) \cap \mathbb{R}$. If*

$$a < \min \left\{ \sqrt{3}\pi/[2N(N-1+2Z)], a_1(\xi) \right\},$$

where $a_1(\xi)$ is defined by (29), then $\xi \in \text{Res}(H_{N,Z}^a)$ and

$$(30) \quad \begin{aligned} & \| (H_{N,Z}^a - \xi)^{-1} - (H_{\text{eff}}^a - \xi)^{-1} \oplus 0 \| \\ & \leq \frac{1}{d_{\text{eff}}(\xi)} \left[\frac{8N}{\sqrt{3}\pi} (N-1+2Z) + C_3(N, Z) \max \left\{ 1, \frac{-\mu}{d_{\text{eff}}(\xi)} \right\} \right] a + \frac{2a^2}{3\pi^2}, \end{aligned}$$

where

$$C_3(N, Z) := 2C_1(N, Z)^2 \frac{\Gamma(1/4)^4 N^{3/2}}{6\pi^3 \sqrt{-\mu}} \left(Z^2 + \frac{(N-1)^2}{\sqrt{2}} \right)$$

and μ is given by (15).

Proof. We may apply Proposition 6.3 that yields $\xi \notin \sigma(H_{\text{eff}}^a - \mathcal{W}^a(\xi))$. So the assumptions of Proposition 6.1 are fulfilled too. Thus, $\xi \in \text{Res}(H_{N,Z}^a)$. Furthermore (28) holds with $\alpha^2 < 1/2$, which implies

$$\frac{1}{d_{\text{eff}}^{\mathcal{W}}(\xi)} \leq \frac{2}{d_{\text{eff}}(\xi)}.$$

Therefore, we have arrived at the following estimate

$$\begin{aligned} & \| (H_{N,Z}^a - \xi)^{-1} - (H_{\text{eff}}^a - \xi)^{-1} \oplus 0 \| \\ & \leq \| (H_{N,Z}^a - \xi)^{-1} - R_{\text{eff}}^{\mathcal{W}}(\xi) \oplus 0 \| + \| R_{\text{eff}}^{\mathcal{W}}(\xi) - (H_{\text{eff}}^a - \xi)^{-1} \| \\ & \leq \frac{1}{d_{\text{eff}}(\xi)} \left[\frac{8N}{\sqrt{3}\pi} (N-1+2Z) + C_3(N, Z) \max \left\{ 1, \frac{-\mu}{d_{\text{eff}}(\xi)} \right\} \right] a + \frac{2a^2}{3\pi^2}. \end{aligned}$$

□

7. APPROXIMATION OF THE TOTAL HAMILTONIAN BY THE TWO-DIMENSIONAL ATOMIC HAMILTONIAN

Theorem 7.1. *Let $\xi \in \text{Res}(h_{N,Z} + NE_1^a) \cap \mathbb{R}$. If $a > 0$ fulfills*

$$a < a_3(\xi) := \min \left\{ e^{-1}, \sqrt{3}\pi/[2N(N-1+2Z)], \tilde{a}_0(\xi - NE_1^a), a_2(\xi) \right\},$$

where $\tilde{a}_0(\xi)$ is defined by (16) and $a_2 = a_2(\xi)$ is the solution to

$$C_3(N, Z) \max \left\{ 1, \frac{-2\mu}{d_{N,Z}(\xi - NE_1^a)} \right\} a_2 = 1$$

with μ given by (15), then $\xi \in \text{Res}(H_{N,Z}^a)$ and

$$\begin{aligned} & \| (H_{N,Z}^a - \xi)^{-1} - (h_{N,Z} + NE_1^a - \xi)^{-1} \oplus 0 \| \\ & \leq \frac{2}{d_{N,Z}(\xi - NE_1^a)} \max \left\{ 1, \frac{-\mu}{d_{N,Z}(\xi - NE_1^a)} \right\} C_1(N, Z)^2 C_2(N, Z) a |\ln a| \\ & + \frac{2}{d_{N,Z}(\xi - NE_1^a)} \left[\frac{8N}{\sqrt{3}\pi} (N-1+2Z) + C_3(N, Z) \max \left\{ 1, \frac{-2\mu}{d_{N,Z}(\xi - NE_1^a)} \right\} \right] a + \frac{2a^2}{3\pi^2}. \end{aligned}$$

Proof. Due to the bound on a we may apply Theorem 5.3 with $\xi - NE_1^a$ substituted for ξ . It implies that $\xi \in \text{Res}(H_{\text{eff}}^a)$ and

$$\begin{aligned} (31) \quad & \| (H_{\text{eff}}^a - \xi)^{-1} - (h_{N,Z} + NE_1^a - \xi)^{-1} \| \\ & \leq \frac{2}{d_{N,Z}(\xi - NE_1^a)} \max \left\{ 1, \frac{-\mu}{d_{N,Z}(\xi - NE_1^a)} \right\} C_1(N, Z)^2 C_2(N, Z) a |\ln a|. \end{aligned}$$

Moreover, by Remark 5.4,

$$(32) \quad \frac{1}{d_{\text{eff}}(\xi)} \leq \frac{2}{d_{N,Z}(\xi - NE_1^a)}.$$

Therefore, $a_2(\xi) \leq a_1(\xi)$, so the assumptions of Theorem 6.4 are also fulfilled. Thus we have $\xi \in \text{Res}(H_{N,Z}^a)$. Observe that

$$\begin{aligned} (33) \quad & \| (H_{N,Z}^a - \xi)^{-1} - (h_{N,Z} + NE_1^a - \xi)^{-1} \oplus 0 \| \leq \| (H_{N,Z}^a - \xi)^{-1} - (H_{\text{eff}}^a - \xi)^{-1} \oplus 0 \| \\ & + \| (H_{\text{eff}}^a - \xi)^{-1} - (h_{N,Z} + NE_1^a - \xi)^{-1} \|. \end{aligned}$$

Putting this together with (30), (31), and (32) finishes the proof. \square

Remark 7.2. *If we set $\xi = NE_1^a + \delta$ with some fixed $\delta \in \text{Res}(h_{N,Z})$, then a_3 does not depend on the parameter a , in fact it depends only on $d_{N,Z}(\delta)$.*

8. PROPERTIES OF THE EIGENVALUES

8.1. Localization. Suppose there is an isolated eigenvalue of $h_{N,Z}$ with a finite multiplicity, let us say λ . If we set $\xi_+ := NE_1^a + \lambda + d$ with $0 < d < \text{dist}(\lambda, \sigma(h_{N,Z}) \setminus \{\lambda\})/2$, then $d_{N,Z}(\xi_+ - NE_1^a) = d$ and in the view of Theorem 7.1 and Remark 7.2 there is $a_{\min}(d) > 0$ such that for all $a < a_{\min}(d)$ we have

$$(34) \quad \| (H_{N,Z}^a - \xi_+)^{-1} - (h_{N,Z} + NE_1^a - \xi_+)^{-1} \oplus 0 \| \leq K(d) a |\ln a|.$$

Let us stress that the value of $K(d) \in \mathbb{R}_+$, as well as that of $a_{\min}(d)$, depends only on d , N , and Z , but not on the particular eigenvalue λ or the value of a .

Furthermore, let Γ stands for the anti-clockwise oriented circle with center $NE_1^a + \lambda$ and radius d . Following the same reasoning as in the concluding remarks of [2] we can propagate (34) to all $\xi \in \Gamma$,

$$\|(H_{N,Z}^a - \xi)^{-1} - (h_{N,Z} + NE_1^a - \xi)^{-1} \oplus 0\| \leq \frac{9K(d)a|\ln a|}{1 - 6dK(d)a|\ln a|}$$

(for a small enough so that $6dK(d)a|\ln a| < 1$). Consequently we arrive at the following estimate for the difference of the projections \mathcal{P}_1 and \mathcal{P}_2 onto the spectrum of $H_{N,Z}^a$ and $h_{N,Z} + NE_1^a$, respectively, inside Γ

$$(35) \quad \begin{aligned} \|\mathcal{P}_1 - \mathcal{P}_2 \oplus 0\| &= \frac{1}{2\pi} \left\| \int_{\Gamma} (H_{N,Z}^a - \xi)^{-1} - (h_{N,Z} + NE_1^a - \xi)^{-1} \oplus 0 \, d\xi \right\| \\ &\leq \frac{9dK(d)a|\ln a|}{1 - 6dK(d)a|\ln a|}. \end{aligned}$$

The RHS of (35) is strictly increasing on some sufficiently small right neighborhood of 0 and it tends to zero as $a \rightarrow 0+$. Consequently $\tilde{a}_{\min}(d)$ exists, $0 < \tilde{a}_{\min}(d) \leq a_{\min}(d)$, such that for all $a < \tilde{a}_{\min}(d)$,

$$\|\mathcal{P}_1 - \mathcal{P}_2 \oplus 0\| < 1.$$

Therefore, for these values of a , in the d -neighborhood of $(\lambda + NE_1^a)$ there is the exactly same number of eigenvalues (counting multiplicity) of $H_{N,Z}^a$ as the multiplicity of λ in the spectrum of $h_{N,Z}$ is.

The idea above may be applied on a finite cluster of successive eigenvalues, $\lambda_1 \dots, \lambda_M$, of $h_{N,Z}$. We just take d sharply smaller than a half of the minimum of isolation distances of all λ_i . Moreover we may perform the similar estimates as above on intervals $[\lambda_i + d, \lambda_{i+1} - d]$ (in particular we change λ for $(\lambda_{i+1} + \lambda_i)/2$ and d for $(\lambda_{i+1} - \lambda_i)/2 - d$) to conclude that for a sufficiently small there are no eigenvalues of $H_{N,Z}^a$ in these intervals.

8.2. Analyticity. Consider a unitary mapping $U_a : L^2(\Omega_a)^{\otimes N} \rightarrow L^2(\Omega_1)^{\otimes N}$ acting as

$$(U_a \psi)(\mathbf{x}_1, \dots, \mathbf{x}_N) = a^{3/2} \psi(a\mathbf{x}_1, \dots, a\mathbf{x}_N),$$

then

$$U_a H_{N,Z}^a U_a^\dagger = \frac{1}{a^2} \left(-\Delta - \sum_{i=1}^N \frac{aZ}{r_i} + \sum_{i < j}^N \frac{a}{r_{i,j}} \right) = \frac{1}{a^2} (-\Delta + a\mathcal{V}) =: \tilde{H}_{N,Z}^a.$$

Observe that

- For all $a > 0$, $\text{Dom}(\tilde{H}_{N,Z}^a) = (\mathcal{H}_0^1(\Omega_1) \cap \mathcal{H}^2(\Omega_1))^{\otimes N} = \text{Dom}(-\Delta) =: \mathcal{D}$. We can also extend the definition of this operator to $a \in \mathbb{C} \setminus \{0\}$. It is well defined on \mathcal{D} due to the Hardy inequality.
- For all $a_0 \neq 0$ and $\psi \in \mathcal{D}$, $\tilde{H}_{N,Z}^{a_0} \psi$ has a derivative with respect to a ,

$$\frac{2}{a_0^3} \Delta \psi - \frac{1}{a_0^2} \mathcal{V} \psi \in L^2(\Omega_1)^{\otimes N},$$

and so $a \mapsto \tilde{H}_{N,Z}^a$ is analytic.

- For $a \in \mathbb{C}$, (6) implies

$$(36) \quad \|a\mathcal{V}\| \leq |a| (2Z^2N + N(N-1)^2)^{1/2} (\epsilon\|-\Delta\psi\| + \epsilon^{-1}\|\psi\|).$$

Thus $a\mathcal{V}$ is infinitesimally $-\Delta$ -bounded. As $-\Delta$ is closed, the same holds true for the first operator (see e.g. [11, Theorem IV.1.1] for a simple proof).

- From (36) it follows

$$\|a\mathcal{V}\| \leq |a| (2Z^2N + N(N-1)^2)^{1/2} (\epsilon\|(-\Delta - \xi)\psi\| + (\epsilon^{-1} + \epsilon|\xi|)\|\psi\|).$$

If $\xi < NE_1^1 = N\pi^2$ then $\xi \in \text{Res}(-\Delta)$. [11, Theorem IV.1.16] says that ξ also belongs to the resolvent set of $-\Delta + a\mathcal{V}$ whenever

$$|a| (2Z^2N + N(N-1)^2)^{1/2} ((\epsilon^{-1} + \epsilon|\xi|)\|(-\Delta - \xi)^{-1}\| + \epsilon) < 1.$$

Since $\|(-\Delta - \xi)^{-1}\| = (N\pi^2 - \xi)^{-1}$ this can be achieved with $\epsilon = |\xi|^{-1/2}$ and ξ sufficiently negative. Thus the resolvent set of $\tilde{H}_{N,Z}^a$ is non-empty.

So here comes the main result of the section.

Proposition 8.1. *$\tilde{H}_{N,Z}^a$ forms an analytic family of type (A) on $\mathbb{C} \setminus \{0\}$ and consequently it forms an analytic family in the sense of Kato, see [20, Theorem XII.9].*

Consequently the (analyticity) statement [20, Theorem XII.8] holds for the non-degenerate isolated eigenvalues of the operator $H_{N,Z}^a$. In particular it says that if, for some $a_0 > 0$, there is an non-degenerate isolated eigenvalue of $H_{N,Z}^{a_0}$, then for a near a_0 there is exactly one isolated non-degenerate eigenvalue of $H_{N,Z}^a$ near this eigenvalue of $H_{N,Z}^{a_0}$.

Remark 8.2 (Monotonicity of the eigenvalues). *In the exactly same manner as in [4], one can prove that the eigenvalues of $H_{N,Z}^a$ (if there are some) are strictly decreasing functions of a .*

9. REDUCTION ON FERMIONIC SUBSPACE

As the physical electrons are fermions, we should reduce the Hamiltonian $H_{N,Z}^a$ to the fermionic subspace $\wedge^N L^2(\Omega_a)$ (the symbol \wedge stands for the antisymmetric tensor product). To do so we introduce a projection P^{AS} on $L^2(\Omega_a)^{\otimes N}$ as follows,

$$(P^{AS}\psi)(\mathbf{r}_1, \dots, \mathbf{r}_N) = \frac{1}{N!} \sum_{\sigma \in S_N} \text{sgn } \sigma \psi(\mathbf{r}_{\sigma(1)}, \dots, \mathbf{r}_{\sigma(N)}).$$

Remark that this projection commutes with $H_{N,Z}^a$, i.e. $P^{AS}H_{N,Z}^a \subset H_{N,Z}^a P^{AS}$. On $\text{Dom}(H_{N,Z}^a)$, we define the 'fermionized' version of Hamiltonian $H_{N,Z}^a$ by

$$H_{N,Z,f}^a := P^{AS}H_{N,Z}^a P^{AS} = H_{N,Z}^a P^{AS}.$$

It is convenient to view $H_{N,Z,f}^a$ as a restriction of $H_{N,Z}^a$ to $P^{AS}\text{Dom}(H_{N,Z}^a)$ acting on

$$P^{AS}L^2(\Omega_a)^{\otimes N} \equiv \wedge^N L^2(\Omega_a).$$

Then $H_{N,Z,f}^a$ is self-adjoint due to the following observation.

Lemma 9.1. *Let H be a self-adjoint operator on a Hilbert space \mathcal{H} and P be an orthogonal projection on \mathcal{H} . If*

- (1) $P\text{Dom}(H)$ is dense in $P\mathcal{H}$
- (2) $PH \subset HP$,

then $H_P := H|_{P\text{Dom}(H)}$ is self-adjoint on $P\mathcal{H}$.

Proof. From the first condition and the self-adjointness of H , it follows $H_P \subset H_P^\dagger$. Next we have $\text{Ran}(H_P \pm i) = P\text{Ran}(H \pm i)$ due to the second condition. But $\text{Ran}(H \pm i) = \mathcal{H}$ by the self-adjointness criterion. By the same criterion we arrive at the assertion of the lemma. \square

Similarly we define the fermionized versions of H_{eff}^a and $h_{N,Z}$ on domains $\text{Dom}(H_{\text{eff}}^a)$ and $\text{Dom}(h_{N,Z})$, respectively,

$$\begin{aligned} H_{\text{eff},f}^a &= P^{AS} P^a H_{N,Z}^a P^a P^{AS} = P^a H_{N,Z}^a P^a P^{AS} \\ h_{N,Z,f} &= P_{2D}^{AS} h_{N,Z} P_{2D}^{AS} = h_{N,Z} P_{2D}^{AS}, \end{aligned}$$

where P_{2D}^{AS} acts in the same manner as P^{AS} but on the Hilbert space $L^2(\mathbb{R}^2)^{\otimes N}$. The operator $H_{\text{eff},f}^a$ may be viewed as acting on $\wedge^N L^2(\mathbb{R}^2)$ with the domain $P_{2D}^{AS} \text{Dom}(H_{\text{eff}}^a)$ and the same action as H_{eff}^a . An analogical statement holds true for $h_{N,Z,f}$. Self-adjointness of $H_{\text{eff},f}^a$ and $h_{N,Z,f}$ then again follows from Lemma 9.1. Moreover, $H_{\text{eff},f}^a$ and $h_{N,Z,f}$ are bounded below with bounds above the lower bounds of H_{eff}^a and $h_{N,Z}$, respectively. In particular we have

$$h_{N,Z,f} \geq \mu + 1, \quad H_{\text{eff},f}^a - NE_1^a \geq \mu + 1$$

with μ given by (15).

Going carefully through the proofs of Theorems 5.3, 6.4, and 7.1 (and the related lemmas) one concludes that these theorems remain valid for the fermionized versions of operators too, if we everywhere interchange $d_{\text{eff}}(\xi)$ and $d_{N,Z}(\xi)$ for $d_{\text{eff},f}(\xi)$ and $d_{N,Z,f}(\xi)$, respectively. Here we introduced

$$d_{\text{eff},f}(\xi) = \text{dist}(\xi, \sigma(H_{\text{eff},f}^a)), \quad d_{N,Z,f}(\xi) = \text{dist}(\xi, \sigma(h_{N,Z,f})).$$

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REFERENCES

- [1] Bouzouina A 2002 Stability of the two-dimensional Brown-Ravenhall operator *Proc. Roy. Soc. Edinburgh Sect. A* **132** 1133–1144
- [2] Brummelhuis R and Duclos P 2006 Effective Hamiltonians for atoms in very strong magnetic fields *J. Math. Phys.* **47** 032103
- [3] Chaos-Cador L and Ley-Koo E 2005 Two-dimensional hydrogen atom confined in circles, angles, and circular sectors *International Journal of Quantum Chemistry* **103** (4) 369–387
- [4] Duclos P and Høegreave H 2010 Hydrogenic system confined by infinite tubes *J. Phys. A* **43** 474018
- [5] De Groot S R, Ten Seldam C A 1946 On the energy levels of a model of the compressed hydrogen atom *Physica* **12** (9-10) 669–682

- [6] Duclos P, Šťovíček P and Tušek M 2010 On the two-dimensional Coulomb-like potential with a central point interaction *J. Phys. A* **43** 474020
- [7] Fröman P O, Yngve S and Fröman N 1987 The energy levels and the corresponding normalized wave functions for a model of a compressed atom *J. Math. Phys.* **28** 1813-26
- [8] Grimaldi C 2008 Energy levels of a two-dimensional hydrogen atom with spin-orbit Rashba interaction *Phys. Rev. B* **77** 113308
- [9] Herbst I W 1977 Spectral theory of the operator $(p^2 + m^2)^{1/2} - Ze^2/r$ *Commun. Math. Phys.* **53** 285–294
- [10] Jaskólski W 1996 Confined many-electrons systems *Phys. Rep.* **271** (1) 1–66
- [11] Kato T 1966 *Perturbation theory for linear operators* New York: Springer-Verlag
- [12] Killingbeck J B 2009 A Hill-series approach to wavefunction nodes *J. Phys. A* **42** 085302
- [13] Laughlin C, Burrows B L and Cohen M 2002 A hydrogen-like atom confined within an impenetrable spherical box *J. Phys. B* **35** 701
- [14] Lima R P A, Amado M and Domínguez-Adame F 2008 A solvable model of hydrogenic impurities in quantum dots *Nanotechnology* **19** 135402
- [15] Michels A, De Boer J and Bijl A 1937 Remarks concerning molecular interaction and their influence on the polarisability *Physica* **4** 981
- [16] Parfitt D G W and Portnoi M E 2002 The two-dimensional hydrogen atom revisited *J. Math. Phys.* **43** 4681
- [17] Nam P T, Portmann F and Solovej J P 2012 Asymptotics for two-dimensional atoms *Ann. H. Poincaré* **13** 333–362
- [18] Reed M and Simon B 1975 *Methods of Modern Mathematical Physics II* New York: Academic Press
- [19] Reed M and Simon B 1979 *Methods of Modern Mathematical Physics III* New York: Academic Press
- [20] Reed M and Simon B 1978 *Methods of Modern Mathematical Physics IV* New York: Academic Press
- [21] Robnik M and Romanovski V G 2003 Two-dimensional hydrogen atom in a strong magnetic field *J. Phys. A* **36** 7923
- [22] Simon B 1977 Geometric Methods in Multiparticle Quantum Systems *Commun. Math. Phys.* **55** 259–274
- [23] Varshni Y P 1999 Accurate wavefunctions for hydrogenic donors in GaAs-(Ga,Al) as quantum dots *Phys. Lett. A* **252** (5) 248–250
- [24] Wang Z Q and Zhu M 2003 Hardy inequalities with boundary terms *Electronic J. Diff. Equations* **43**, 1–8
- [25] Yang X L, Guo S H, Chan F T, Wong K W and Ching W Y 1991 Analytic solution of a two-dimensional hydrogen atom. I. Non-relativistic theory *Phys. Rev. A* **43** 1186–1205

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